

=> fil hcaplu

FILE 'HCAPLUS' ENTERED AT 12:35:08 ON 05 FEB 2003

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FILE COVERS 1907 - 5 Feb 2003 VOL 138 ISS 6

FILE LAST UPDATED: 4 Feb 2003 (20030204/ED)

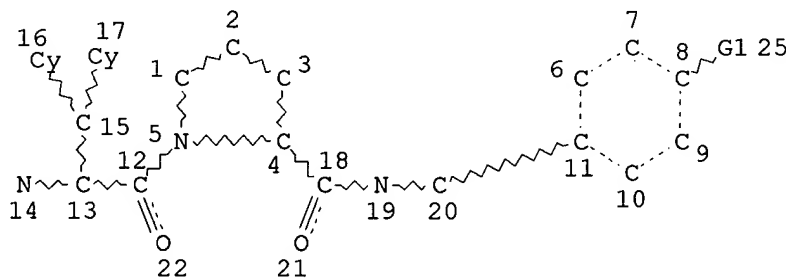
This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3

STR

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VAR G1=N/23

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L5 55 SEA FILE=REGISTRY SSS FUL L3

L6 7 SEA FILE=HCAPLUS L5

=> d ibib abs hitrn l6 1-7

L6 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:490612 HCAPLUS

DOCUMENT NUMBER: 137:185834

TITLE: Preparation of peptidic thrombin inhibitor showing

Searched by M. Smith

INVENTOR(S): distinguished oral absorption  
Park, Cheol Won; Lee, Gu; Lee, Sang Gu; Lee, Seung  
PATENT ASSIGNEE(S): LG Chemical Co., Ltd., S. Korea  
SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given  
CODEN: KRXXA7  
DOCUMENT TYPE: Patent  
LANGUAGE: Korean  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2000052621	A	20000825	KR 1999-64851	19991229
US 2002169113	A1	20021114	US 2001-810243	20010319
PRIORITY APPLN. INFO.:			KR 1998-60265	A 19981229
			KR 1998-60267	A 19981229

AB A peptidic thrombin inhibitor compn. showing distinguished oral-absorption is provided, which shows excellent thrombus prodn. inhibiting effect, so which can be used for preventing blood coagulation and treating various thrombosis. A process for the prepn. of (2S)-N-[4-[amino(imino)methyl]benzyl]-1-[(2R)-2-[(aminosulfonyl)amino]-3,3-diphenylpropanoyl]-2-pyrrolidinecarboxamide trifluoroacetate (TFA) (I) comprises of: (a) prepg. H2NSO2-D-diphenylalanine(Dpa)-L-proline(Pro)-OMe (II) by adding sulfamoyl chloride and trimethylamine to H-D-Dpa-Pro-OMe.HCl dichloromethane soln.; (b) prepg. H2NSO2-D-Dpa-Pro-OH (III) by suspending the compd. II to water and methanol, adding LiOH soln., shaking, and filtering; (c) manufg. HN2SO2-D-Dpa-Pro-(4-CNbenzyl)amide (IV) by dissolving the compd. III in DMF, cooling, adding 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide.HCl and 1-hydroxybenzotriazole hydrate, adding 4-cyanobenzylamine.HCl and N-methylmorpholine; and (d) dissolving the compd. IV in pyridine, adding trimethylamine, satg. with H2S gas, removing volatile material, drying, adding acetone, iodomethane, removing volatile material, drying, dissolving the residue with acetonitrile, adding ammonium acetate, concg., and refining to get the objective compd. I.

IT 451455-55-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide as thrombin inhibitor with distinguished oral absorption)

IT 451455-56-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of peptide as thrombin inhibitor with distinguished oral absorption)

L6 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:211221 HCAPLUS

DOCUMENT NUMBER: 137:241663

TITLE: Noncovalent tripeptidic thrombin inhibitors  
incorporating amidrazone, amine and amidine functions  
at P1

AUTHOR(S): Lee, Koo; Jung, Won-Hyuk; Park, Cheol Won; Park, Hee  
Dong; Lee, Sun Hwa; Kwon, O. Hwan

CORPORATE SOURCE: Life Science R&D, LGCI, Yu-Sung, Science Town, Taejon,  
305-380, S. Korea

Searched by M. Smith

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),  
12(7), 1017-1022  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A series of noncovalent tripeptidic thrombin inhibitors incorporating amidrazone, amine and amidine functions at P1 was investigated. While the amidrazone and the amine series displayed limited oral absorption, the amidine series demonstrated generally good oral absorption and strong antithrombotic activity; the single-digit picomolar  $K_i$  achieved from this series is among the best yet reported. The present work highlights the benzamidine, one of the compds., LB30812 that exhibits excellent overall profiles of potency, oral absorption and antithrombotic efficacy.

IT 451455-55-3 460323-25-5 460323-27-7  
460323-29-9 460323-31-3 460323-33-5  
460323-35-7 460323-37-9 460323-39-1  
460323-41-5

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (noncovalent tripeptidic thrombin inhibitors incorporating amidrazone, amine and amidine functions at P1)

IT 460323-12-0 460323-16-4 460323-17-5  
460323-18-6 460323-20-0

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (noncovalent tripeptidic thrombin inhibitors incorporating amidrazone, amine and amidine functions at P1)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:46504 HCAPLUS

DOCUMENT NUMBER: 137:149706

TITLE: Multiple conformer protocol: A new method for the identification of preferred ligand binding motifs using cross-validated 3D-QSAR models

AUTHOR(S): Doweyko, A. M.

CORPORATE SOURCE: Structural Biology and Modeling, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 09543, USA

SOURCE: Rational Approaches to Drug Design, Proceedings of the European Symposium on Quantitative Structure-Activity Relationships, 13th, Duesseldorf, Germany, Aug. 27-Sept. 1, 2000 (2001), Meeting Date 2000, 307-315. Editor(s): Hoeltje, Hans-Dieter; Sippl, Wolfgang. Prous Science: Barcelona, Spain. CODEN: 69CEP6; ISBN: 84-8124-176-8

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The ability of multiple conformer protocol (MCP) to identify the x-ray crystal structures of bound ligands in the presence of reasonable alternative bound conformers was tested. Thirty-two elastase inhibitors and 28 thrombin inhibitors were subjected to MCP anal. to identify the x-ray coordinates from among 320 conformers and 291 conformers derived from a docking protocol. The MCP represents a new method for the discovery of the most probable coordinates of a series of bound ligand structures by means of intervening cross-validated 3D-QSAR models. The

MCP was able to identify the x-ray crystal structures of bound ligands in two cases: 6 of 7 elastase inhibitors and 6/11 thrombin inhibitors, using relatively small data sets having activity ranges of five orders of magnitude. The use of a 3D-QSAR methodol. such as hypothetical active site lattice (HASL) was a key element in a cross-validation scoring of intermediate subset models. The presence of an external conformational constraint in the form of the protein target or a pharmacophoric/alignment paradigm would seem to be significant, since a truly randomized set of conformers would otherwise present an intractable 3D-QSAR problem. Utilizing, a protein binding site constraint, the MCP has wide applicability in the detn. of preferred ligand binding motifs across chemotypes which enables predictive 3D-QSAR and enhances rational structure-based design.

IT **446063-81-6**

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(multiple conformer protocol, a new method for identification of preferred ligand binding motifs using cross-validated 3D-QSAR models)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:790173 HCAPLUS

DOCUMENT NUMBER: 133:350506

TITLE: Preparation of 2,3-methano-amino acid derivatives as anticoagulant agents

INVENTOR(S): De Nanteuil, Guillaume; Gloanec, Philippe; Verbeuren, Tony; Rupin, Alain

PATENT ASSIGNEE(S): Adir et Compagnie, Fr.

SOURCE: Eur. Pat. Appl., 34 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

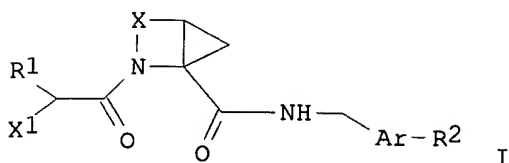
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1050534	A1	20001108	EP 2000-401197	20000502
EP 1050534	B1	20011205		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2793248	A1	20001110	FR 1999-5601	19990503
FR 2793248	B1	20010629		
CN 1277961	A	20001227	CN 2000-119227	20000430
NO 2000002314	A	20001106	NO 2000-2314	20000502
US 6288077	B1	20010911	US 2000-561618	20000502
ES 2169716	T3	20020716	ES 2000-401197	20000502
CA 2308780	AA	20001103	CA 2000-2308780	20000503
ZA 2000002152	A	20001107	ZA 2000-2152	20000503
BR 2000002075	A	20010102	BR 2000-2075	20000503
JP 2000344745	A2	20001212	JP 2000-134144	20000508
JP 3200053	B2	20010820		

PRIORITY APPLN. INFO.: FR 1999-5601 A 19990503

OTHER SOURCE(S): MARPAT 133:350506

GI

Searched by M. Smith



AB Amino acid derivs. I [X = (CH<sub>2</sub>)<sub>n</sub>; n = 2, 3; R1 = cycloalkyl; R2 = amino, alkyl, OH, guanidinoisothiourido; Ar = aryl, heteroaryl; X1 = OH, substituted amine] were prepd. as anticoagulants. Thus, 1-(N-carboxymethyl-(2R)-3-cyclohexylalanyl)-N-(4-amidinobenzyl)-(2S,3R)-2,3-methanoprolinamide hydrochloride was prepd. and tested for its anticoagulant activity (IC<sub>50</sub> = 5.3 .mu.M).

IT **304910-21-2P 304910-23-4P 304910-24-5P**  
**304910-71-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 2,3-methano-amino acid derivs. as anticoagulant agents)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:169727 HCAPLUS

DOCUMENT NUMBER: 128:238973

TITLE: Design of Novel, Potent, Noncovalent Inhibitors of Thrombin with Nonbasic P-1 Substructures: Rapid Structure-Activity Studies by Solid-Phase Synthesis  
AUTHOR(S): Lumma, William C., Jr.; Witherup, Keith M.; Tucker, Thomas J.; Brady, Steven F.; Sisko, John T.; Naylor-Olsen, Adel M.; Lewis, S. Dale; Lucas, Bobby J.; Vacca, Joseph P.

CORPORATE SOURCE: Departments of Medicinal Chemistry Molecular Design and Diversity and Biological Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (1998), 41(7), 1011-1013

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Study of surface representations of the inhibitor-bound thrombin P-1 pocket revealed a lipophilic recess in this pocket which is not occupied by any known inhibitor. Solid-phase synthesis was used to generate benzylamides of D-diphenylAlaPro by ammonolysis of Boc dipeptide Kaiser resin. The resulting amides inhibited thrombin in the range IC<sub>50</sub> = 3-13 000 nM, and the structure-activity relationships and mol. modeling suggest a unique fit of the benzyl side chain into P-1 with the meta substituent occupying the recess.

IT **204975-29-1P 204975-30-4P 204975-31-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(design of novel, potent, noncovalent inhibitors of thrombin with nonbasic P-1 substructures via rapid structure-activity studies by solid-phase synthesis)

Searched by M. Smith

L6 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:632101 HCAPLUS

DOCUMENT NUMBER: 125:301605

TITLE: Preparation of dipeptide amidine analogs as thrombin inhibitors.

INVENTOR(S): Boehm, Hans-Joachim; Hoeffken, Hans Wolfgang;  
Hornberger, Wilfried; Koser, Stefan; Mack, Helmut;  
Pfeiffer, Thomas; Seitz, Werner; Zierke, Thomas

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: PCT Int. Appl., 152 pp.

CODEN: PIXXD2

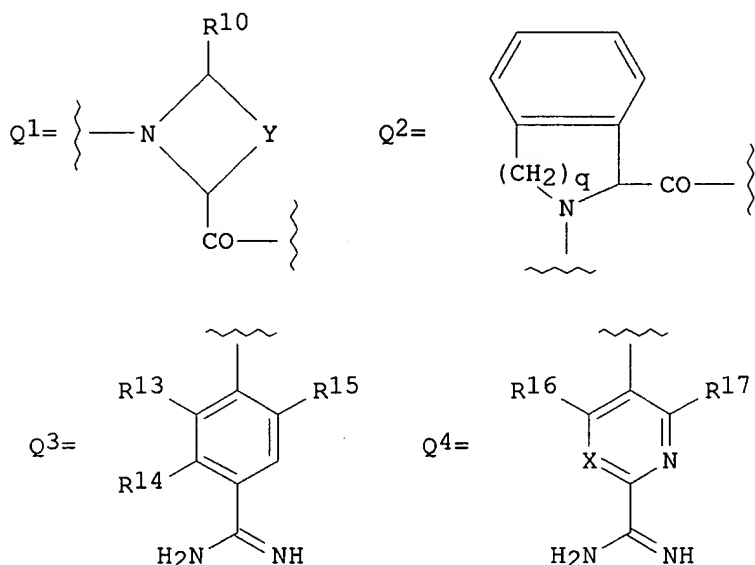
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625426	A1	19960822	WO 1996-EP582	19960212
W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, AZ, BY, KG, KZ, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2211109	AA	19960822	CA 1996-2211109	19960212
AU 9648751	A1	19960904	AU 1996-48751	19960212
AU 708001	B2	19990729		
CN 1175953	A	19980311	CN 1996-191967	19960212
BR 9607582	A	19980707	BR 1996-7582	19960212
EP 873356	A1	19981028	EP 1996-904759	19960212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
JP 11500120	T2	19990106	JP 1996-524648	19960212
TW 450968	B	20010821	TW 1996-85102085	19960216
ZA 9601276	A	19970819	ZA 1996-1276	19960219
US 6030972	A	20000229	US 1997-894252	19970730
FI 9703360	A	19970815	FI 1997-3360	19970815
NO 9703764	A	19971015	NO 1997-3764	19970815
US 6444817	B1	20020903	US 1999-414681	19991008
US 2002169318	A1	20021114	US 2002-100099	20020319
PRIORITY APPLN. INFO.:			DE 1995-19505484 A	19950217
			DE 1995-19506611 A	19950224
			DE 1995-19507455 A	19950303
			WO 1996-EP582 W	19960212
			US 1997-894252 A3	19970730
			US 1999-414681 A3	19991008
OTHER SOURCE(S):			MARPAT 125:301605	
GI				



AB ABNHCR1R2D [R1 = H, alkyl; R2 = H, alkyl, Ph, phenylalkyl, R18OCH2, R18CO, R18NHCOCO, etc.; R18 = H, alkyl, Ph, phenylalkyl, CF3CO, alkoxycarbonyl, etc.; A = R3R4NCR5[(CH2)mR6]CO, R7O[(CH2)mR8]CO, etc.; m = 0, 1; R3, R4 = H, alkyl, arylalkyl, etc.; R5 = H, alkyl, PhCH2; R6 = (substituted) cycloalkyl, Ph, adamantyl, norbornyl, 1-decalinyl, etc.; R7 = H, alkyl, alkylcarbonyl, aminocarbonyl, aminocarbonylalkyl, 5-tetrazolylmethyl, bile acid acyl residue, etc.; R8 = (substituted) Ph, cycloalkyl, 1-indanyl, dibenzosuberyl, etc.; B = Q1, Q2, R11NCHR12CO, etc.; q = 1, 2; Y = CH2, CH2CH2 such that the resulting ring can have an OH, O, or alkoxy group at the 4-position, CH2S, CH2SO, CH:CH, etc.; R10 = H, alkyl, Ph; R11, R12 = H, alkyl, cycloalkyl, Ph, PhCH2; D = Q3, Q4, etc.; R13-R15 = H, NO2, F, Cl, Br, iodo, cycloalkyl, amino, acylamino, etc.; R13R14 = (CH2)3, (CH2)4, OCH2O, CH:CHCH:CH; R16, R17 = H, F, Cl, alkyl, phenylalkyl, Ph, CO2H, alkoxycarbonyl, amino, etc.; X = CH, N], were prepd. as thrombin inhibitors (no data). Thus, D-3-phenyllactylproline p-amidinogbenzylamide acetate salt was prepd. via coupling of O-tetrahydropyranyl-D-3-phenyllactic acid with N-(p-cyanobenzyl)prolinamide followed by conversion of the cyano function to the thioamide and then thioimide.

IT **182286-35-7P 182286-65-3P 182292-29-1P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of dipeptide amidine analogs as thrombin inhibitors)

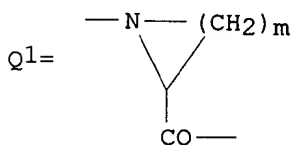
IT **182159-33-7P 182289-23-2P 182289-25-4P**  
**182289-27-6P 182290-29-5P 182290-30-8P**  
**182290-31-9P 182290-33-1P 182292-30-4P**  
**182292-31-5P 182292-32-6P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of dipeptide amidine analogs as thrombin inhibitors)

L6 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1996:623129 HCAPLUS  
 DOCUMENT NUMBER: 125:276585

Searched by M. Smith

TITLE: Preparation of dipeptide amidinobenzylamides and related compounds as thrombin inhibitors.  
INVENTOR(S): Seitz, Werner; Mack, Helmut; Zierke, Thomas; Boehm, Hans-Joachim; Hoeffken, Hans Wolfgang; Koser, Stefan; Pfeiffer, Thomas; Hornberger, Wilfried  
PATENT ASSIGNEE(S): BASF A.-G., Germany  
SOURCE: PCT Int. Appl., 40 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9624609	A1	19960815	WO 1996-EP472	19960206
W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, SG, SK, TR, UA, US, AZ, BY, KG, KZ, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19504504	A1	19960814	DE 1995-19504504	19950210
DE 19506610	A1	19960829	DE 1995-19506610	19950224
AU 9647875	A1	19960827	AU 1996-47875	19960206
AU 706834	B2	19990624		
EP 809651	A1	19971203	EP 1996-903987	19960206
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
BR 9607412	A	19980707	BR 1996-7412	19960206
JP 10513462	T2	19981222	JP 1996-523967	19960206
US 5932567	A	19990803	US 1997-875515	19970730
FI 9703282	A	19970808	FI 1997-3282	19970808
NO 9703657	A	19971003	NO 1997-3657	19970808
PRIORITY APPLN. INFO.:			DE 1995-19504504	19950210
			DE 1995-19506610	19950224
			WO 1996-EP472	19960206
OTHER SOURCE(S):	MARPAT 125:276585			
GI				



AB R1SO2ABNHDC(:NH)NH2 [R1 = OH, alkyl, fluoroalkyl, cycloalkyl, aralkyl, aryl, heteroaryl, etc.; A = NHCR4R5CO; R4 = H, alkyl, cycloalkyl, aryl, aralkyl; R5 = H, alkyl, cycloalkyl, cycloalkylmethyl, bicycloalkyl(methyl), adamantyl(methyl), etc.; B = (substituted) Q1; m = 2-4; D = (substituted) PhCH2, heteroarylmethyl], were prepd. as thrombin inhibitors (no data). Thus, BOC-Pro-OH was coupled with 4-aminomethyl-3-methoxybenzonitrile (prepn. given) using hydroxysuccinimide/DCC in CH2Cl2 to give 65% BOC-Proline (4-cyano-2-methoxy)benzylamide. The latter was deprotected and coupled with BOC-D-Phe(4-OMe)-OH using diisopropylethylamine/propanephosphonic anhydride to give BOC-D-(4-methoxyphenylalanyl)proline (4-cyano-2-methoxy)benzylamide. The latter was elaborated in several steps to title compd. N-methylsulfonyl-D-(4-methoxy)phenylalanylproline



(2-methoxy-4-amidino)benzylamide acetate salt.

IT 182158-97-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide amidinobenzylamides and related compds. as thrombin inhibitors)

IT 182158-96-9P 182159-32-6P 182159-33-7P

182159-34-8P 182159-35-9P 182159-36-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of peptide amidinobenzylamides and related compds. as thrombin inhibitors)

=> fil caold

FILE 'CAOLD' ENTERED AT 12:35:38 ON 05 FEB 2003

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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L7 0 L5

=> fil reg

FILE 'REGISTRY' ENTERED AT 12:35:49 ON 05 FEB 2003

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STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP

Searched by M. Smith

PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

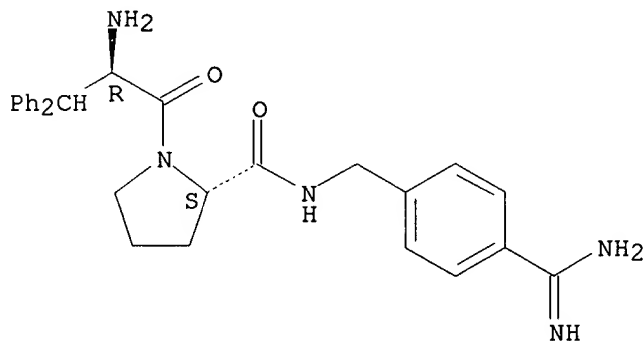
=> d ide can 15 tot

L5 ANSWER 1 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-41-5 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl)methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H31 N5 O2 . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

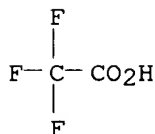
CRN 460323-40-4  
CMF C28 H31 N5 O2

Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

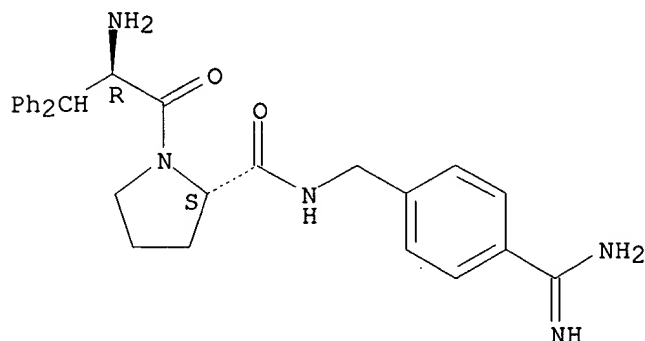
REFERENCE 1: 137:241663

L5 ANSWER 2 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-40-4 REGISTRY

Searched by M. Smith

CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H31 N5 O2  
CI COM  
SR CA

Absolute stereochemistry.



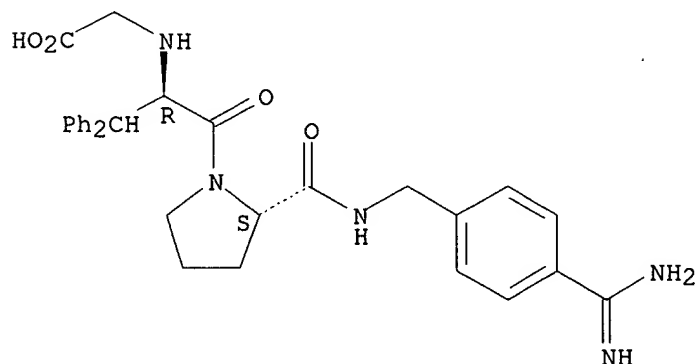
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 3 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-39-1 REGISTRY  
CN L-Prolinamide, N-(carboxymethyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H33 N5 O4 . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-38-0  
CMF C30 H33 N5 O4

Absolute stereochemistry.

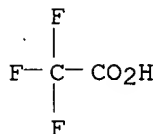


Searched by M. Smith

CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 4 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 460323-38-0 REGISTRY

CN L-Prolinamide, N-(carboxymethyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

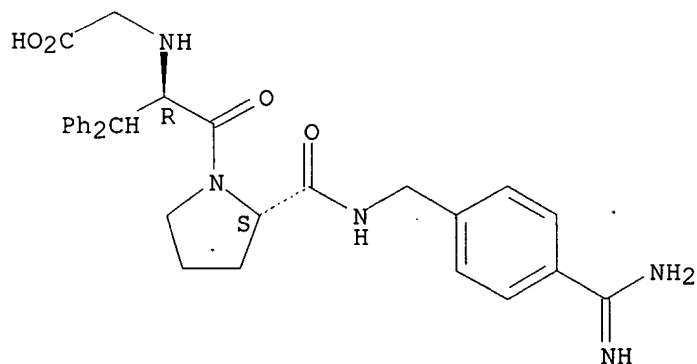
FS STEREOSEARCH

MF C30 H33 N5 O4

CI COM

SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 5 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 460323-37-9 REGISTRY

CN L-Prolinamide, N-(methoxycarbonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H33 N5 O4 . C2 H F3 O2

SR CA

Searched by M. Smith

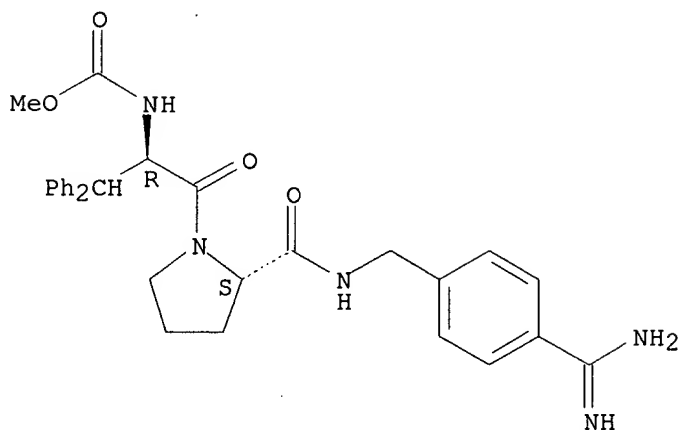
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-36-8

CMF C30 H33 N5 O4

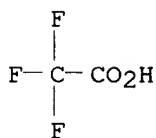
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 6 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 460323-36-8 REGISTRY

CN L-Prolineamide, N-(methoxycarbonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

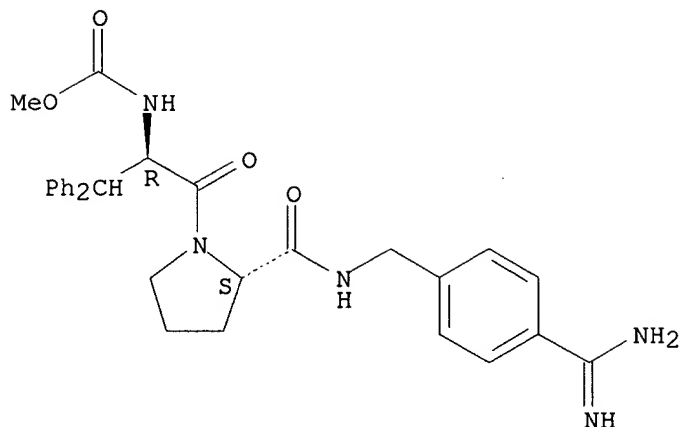
MF C30 H33 N5 O4

CI COM

SR CA

Absolute stereochemistry.

Searched by M. Smith



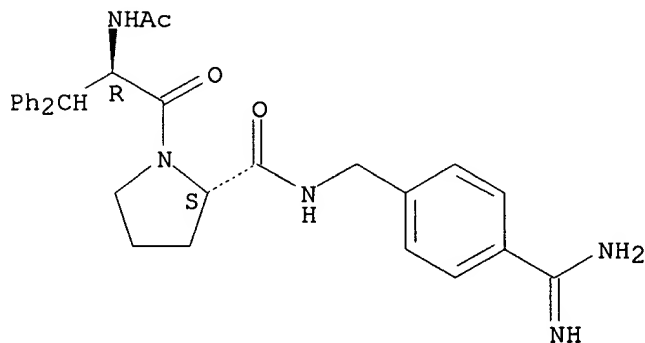
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 7 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-35-7 REGISTRY  
CN L-Prolinamide, N-acetyl-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H33 N5 O3 . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-34-6  
CMF C30 H33 N5 O3

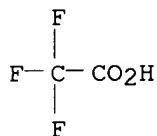
Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2

Searched by M. Smith

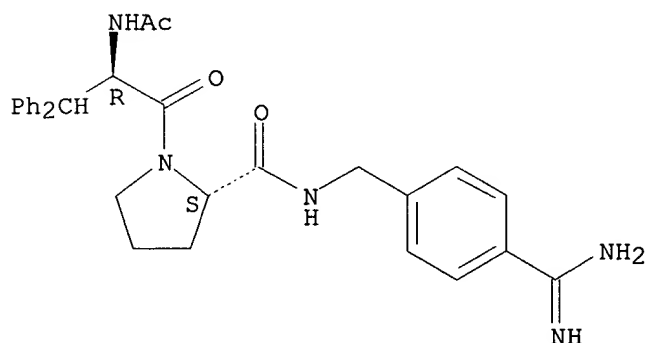


1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 8 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-34-6 REGISTRY  
CN L-Prolinamide, N-acetyl-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H33 N5 O3  
CI COM  
SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

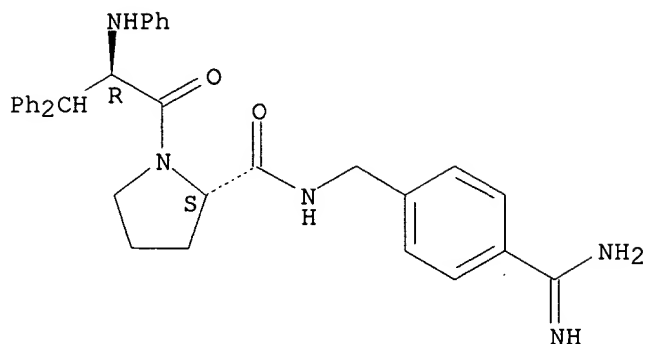
L5 ANSWER 9 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-33-5 REGISTRY  
CN L-Prolinamide, N,.beta.-diphenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H35 N5 O2 . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-32-4  
CMF C34 H35 N5 O2

Searched by M. Smith

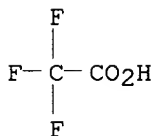
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 10 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 460323-32-4 REGISTRY

CN L-Prolinamide, N,.beta.-diphenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C34 H35 N5 O2

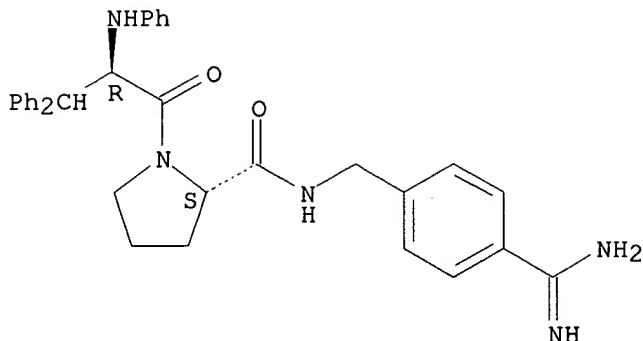
CI COM

SR CA

Absolute stereochemistry.

Searched by M. Smith





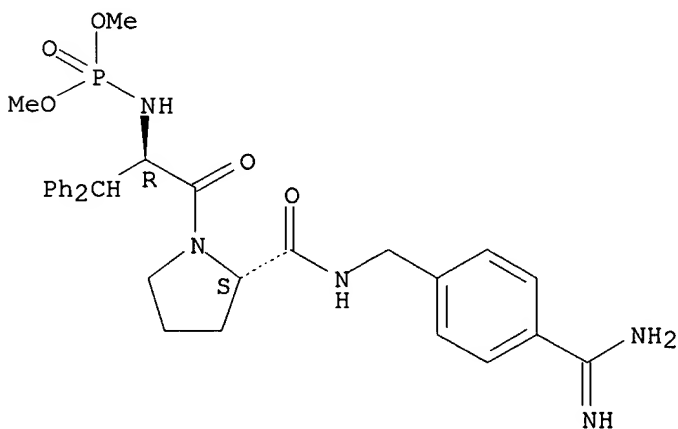
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 11 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-31-3 REGISTRY  
CN L-Prolinamide, N-(dimethoxyphosphinyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H36 N5 O5 P . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-30-2  
CMF C30 H36 N5 O5 P

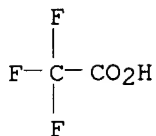
Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2

Searched by M. Smith

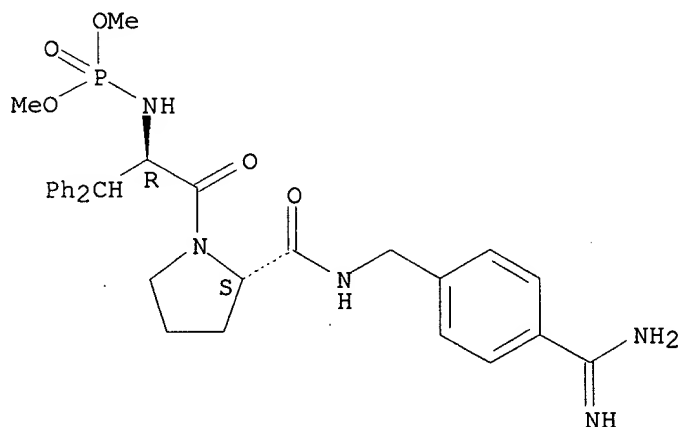


1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 12 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-30-2 REGISTRY  
CN L-Prolinamide, N-(dimethoxyphosphinyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H36 N5 O5 P  
CI COM  
SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

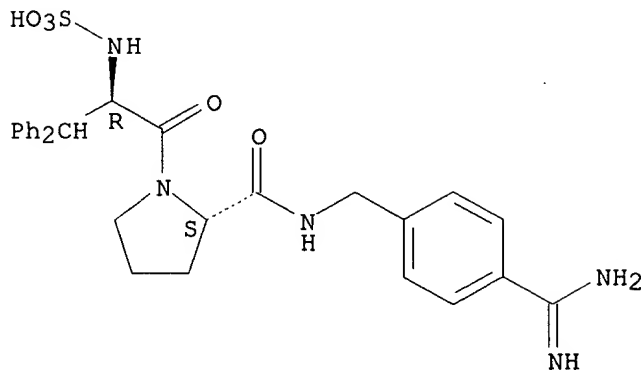
L5 ANSWER 13 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-29-9 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-N-sulfo-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H31 N5 O5 S . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

Searched by M. Smith

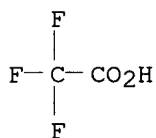
CRN 460323-28-8  
CMF C28 H31 N5 O5 S

Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2



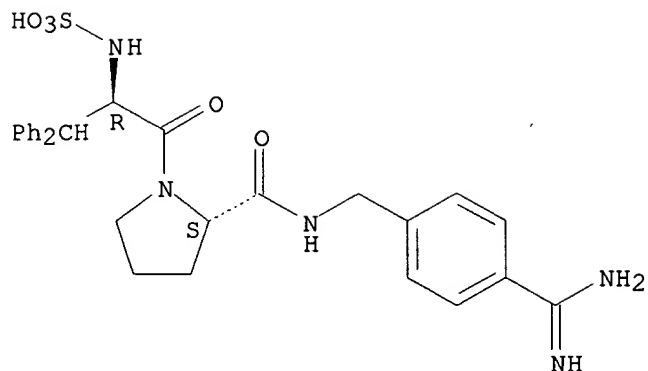
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 14 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-28-8 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-N-sulfo-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H31 N5 O5 S  
CI COM  
SR CA

Absolute stereochemistry.

Searched by M. Smith



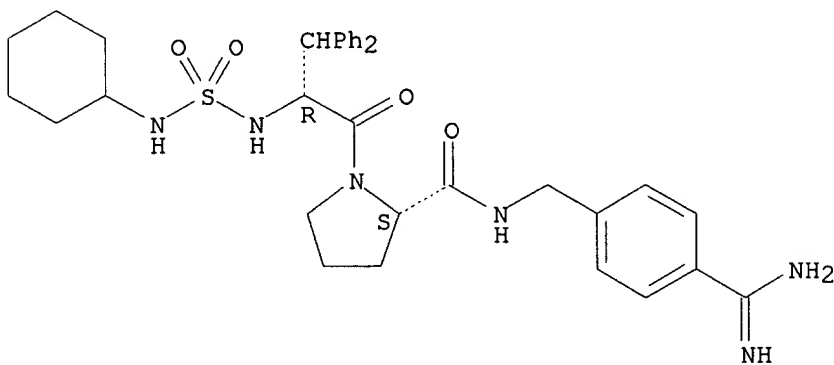
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 15 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-27-7 REGISTRY  
CN L-Prolinamide, N-[(cyclohexylamino)sulfonyl]-.beta.-phenyl-D-phenylalanyl-  
N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C34 H42 N6 O4 S . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-26-6  
CMF C34 H42 N6 O4 S

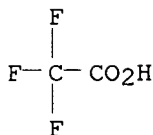
Absolute stereochemistry.



CM 2

CRN 76-05-1  
CMF C2 H F3 O2

Searched by M. Smith

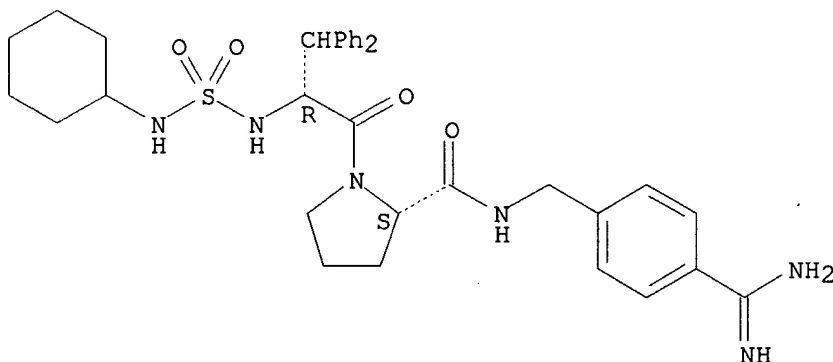


1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 16 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-26-6 REGISTRY  
CN L-Prolinamide, N-[(cyclohexylamino)sulfonyl]-.beta.-phenyl-D-phenylalanyl-  
N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H42 N6 O4 S  
CI COM  
SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

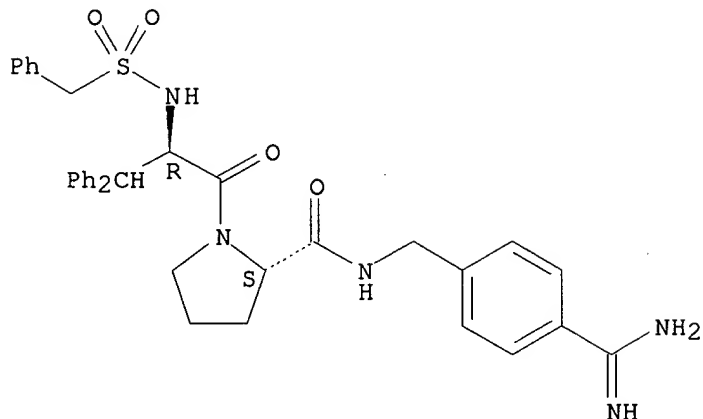
L5 ANSWER 17 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-25-5 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-N-[(phenylmethyl)sulfonyl]-D-phenylalanyl-N-  
[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C35 H37 N5 O4 S . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS

CM 1

CRN 460323-24-4  
CMF C35 H37 N5 O4 S

Searched by M. Smith

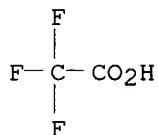
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 18 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 460323-24-4 REGISTRY

CN L-Prolineamide, .beta.-phenyl-N-[(phenylmethyl)sulfonyl]-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

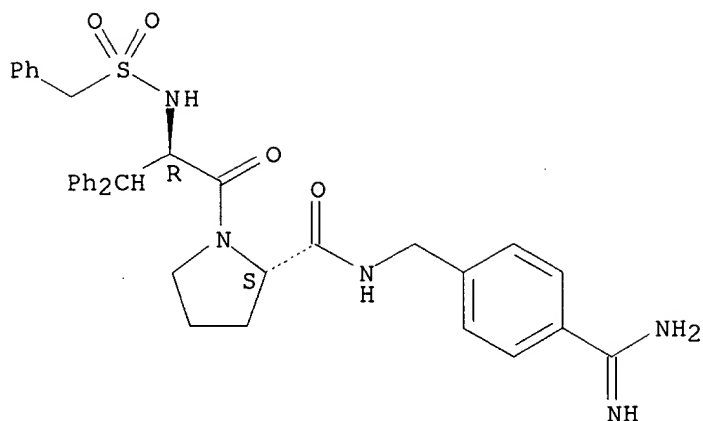
MF C35 H37 N5 O4 S

CI COM

SR CA

Absolute stereochemistry.

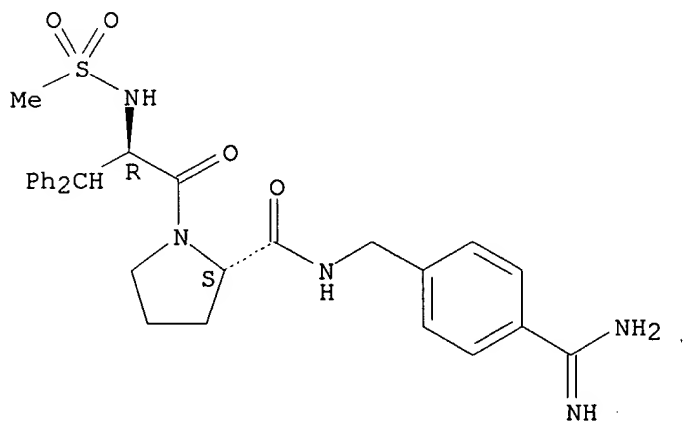
Searched by M. Smith



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 19 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-20-0 REGISTRY  
CN L-Prolineamide, N-(methylsulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H33 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

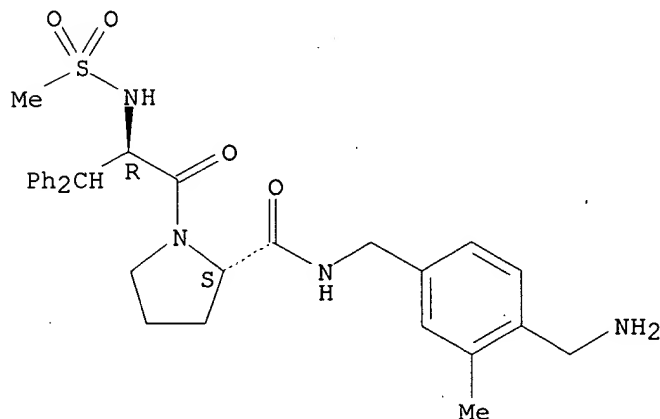
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

Searched by M. Smith

L5 ANSWER 20 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-18-6 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminomethyl)-3-methylphenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H36 N4 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

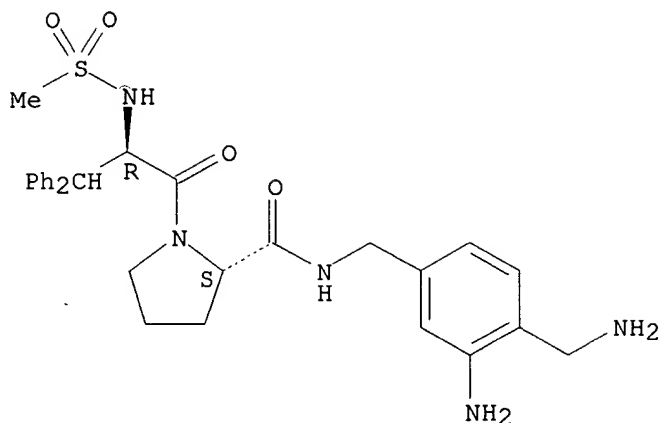
REFERENCE 1: 137:241663

L5 ANSWER 21 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-17-5 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[3-amino-4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H35 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by M. Smith





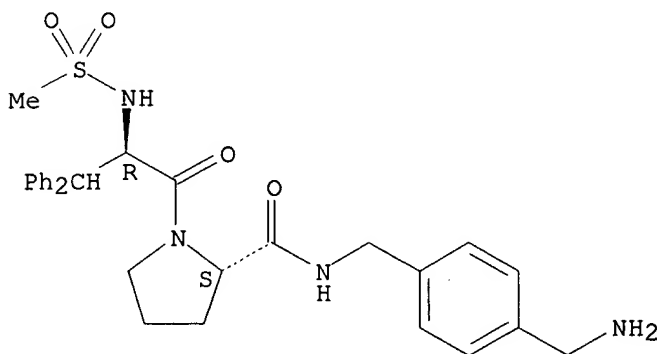
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 22 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-16-4 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H34 N4 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

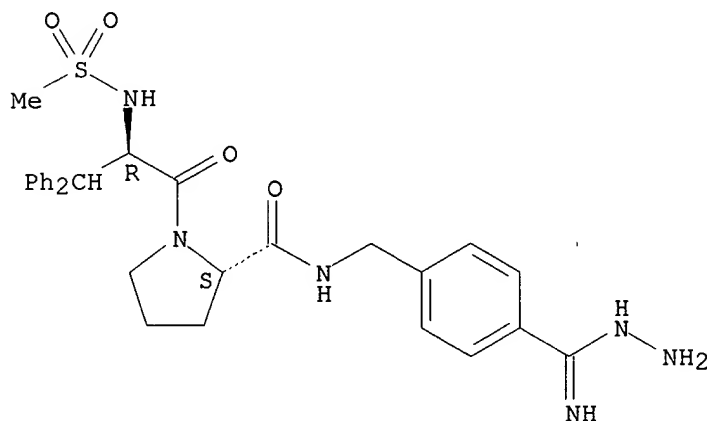
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

Searched by M. Smith

L5 ANSWER 23 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 460323-12-0 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(hydrazinoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H34 N6 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

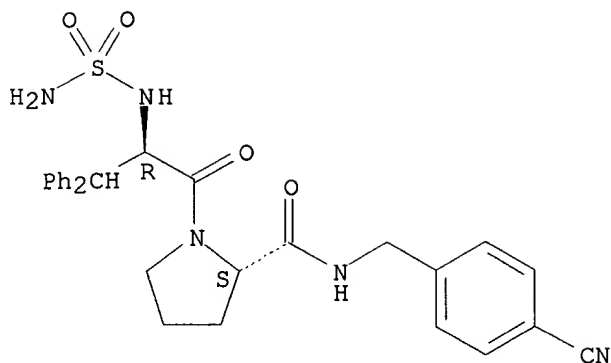
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

L5 ANSWER 24 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 451455-56-4 REGISTRY  
CN L-Prolinamide, N-(aminosulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[(4-cyanophenyl)methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H29 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Searched by M. Smith



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

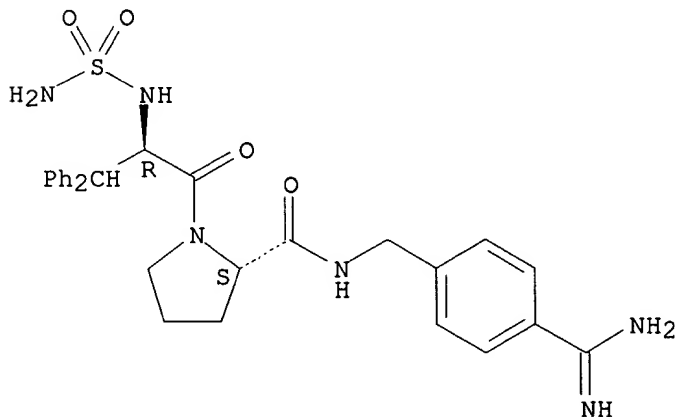
REFERENCE 1: 137:185834

L5 ANSWER 25 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 451455-55-3 REGISTRY  
CN L-Prolinamide, N-(aminosulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H32 N6 O4 S . C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 451455-54-2  
CMF C28 H32 N6 O4 S

Absolute stereochemistry.

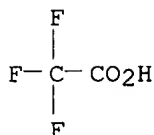


Searched by M. Smith

CM 2

CRN 76-05-1

CMF C2 H F3 O2



2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:241663

REFERENCE 2: 137:185834

L5 ANSWER 26 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 451455-54-2 REGISTRY

CN L-Prolinamide, N-(aminosulfonyl)-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

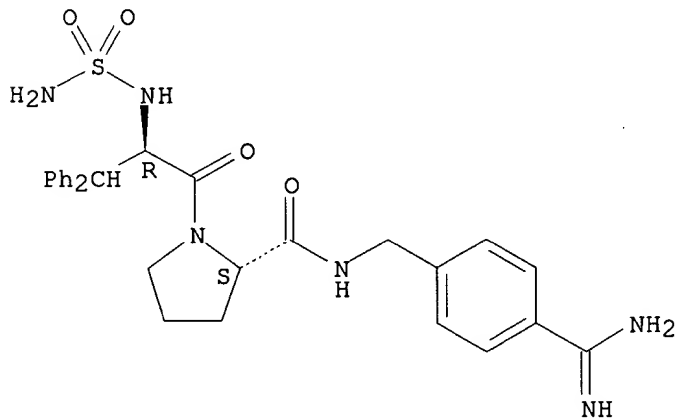
FS STEREOSEARCH

MF C28 H32 N6 O4 S

CI COM

SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 27 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 446063-81-6 REGISTRY

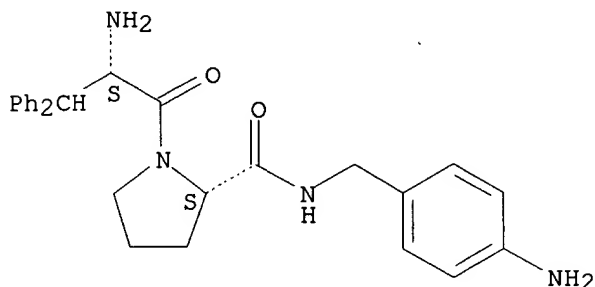
CN L-Prolinamide, .beta.-phenyl-L-phenylalanyl-N-[(4-aminophenyl)methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

Searched by M. Smith

MF C27 H30 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



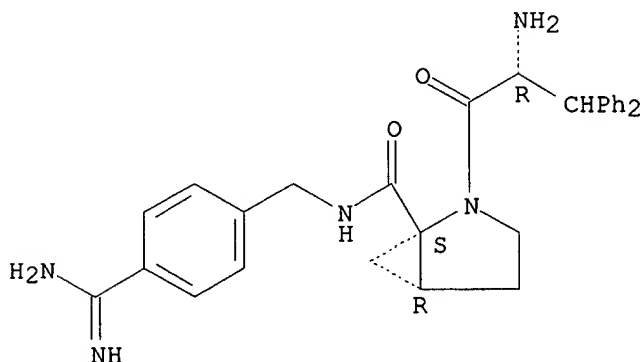
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 137:149706

L5 ANSWER 28 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 304910-71-2 REGISTRY  
CN 2-Azabicyclo[3.1.0]hexane-1-carboxamide, N-[[4-(aminoiminomethyl)phenyl)methyl]-2-[(2R)-2-amino-1-oxo-3,3-diphenylpropyl]-, (1S,5R)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H31 N5 O2  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

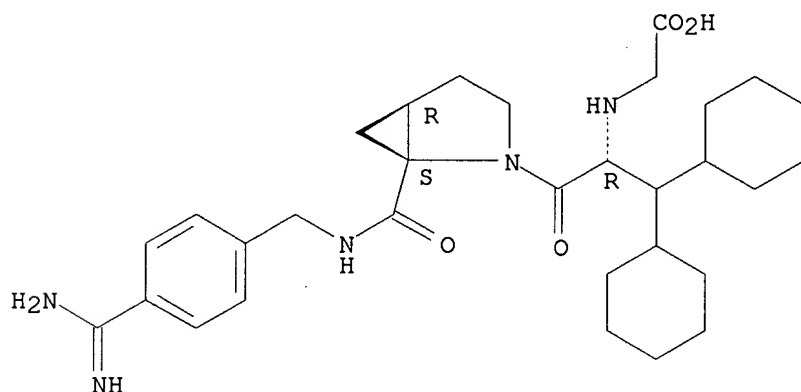
Searched by M. Smith

## 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:350506

L5 ANSWER 29 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 304910-24-5 REGISTRY  
CN Glycine, N-[(1R)-2-[(1S,5R)-1-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-azabicyclo[3.1.0]hex-2-yl]-1-(dicyclohexylmethyl)-2-oxoethyl]-, hydrochloride (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H45 N5 O4 . x Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



● x HCl

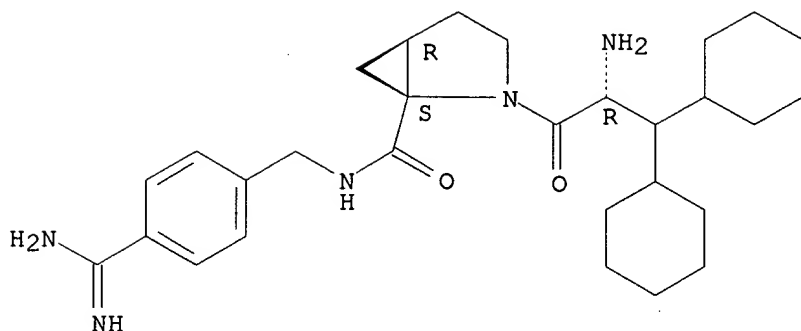
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:350506

L5 ANSWER 30 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 304910-23-4 REGISTRY  
CN 2-Azabicyclo[3.1.0]hexane-1-carboxamide, 2-[(2R)-2-amino-3,3-dicyclohexyl-1-oxopropyl]-N-[[4-(aminoiminomethyl)phenyl]methyl]-, dihydrochloride, (1S,5R)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H43 N5 O2 . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Searched by M. Smith



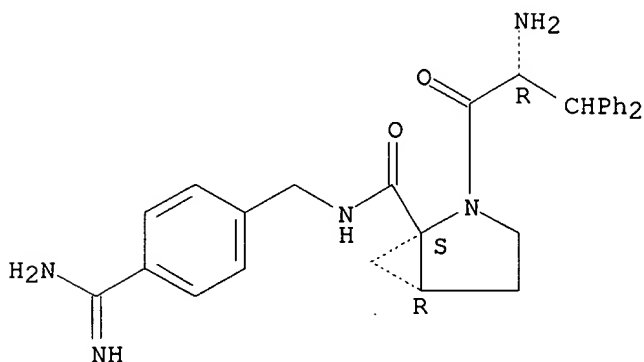
● 2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:350506

L5 ANSWER 31 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 304910-21-2 REGISTRY  
CN 2-Azabicyclo[3.1.0]hexane-1-carboxamide, N-[[4-(aminoiminomethyl)phenyl]methyl]-2-[(2R)-2-amino-1-oxo-3,3-diphenylpropyl]-, dihydrochloride, (1S,5R)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H31 N5 O2 . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
CRN (304910-71-2)

Absolute stereochemistry.



2 HCl

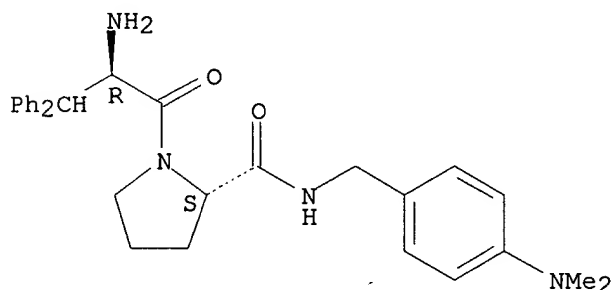
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

Searched by M. Smith

REFERENCE 1: 133:350506

L5 ANSWER 32 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 204975-31-5 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(dimethylamino)phenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H34 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



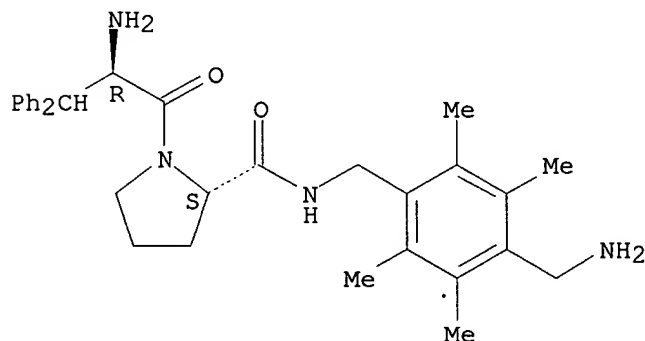
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:238973

L5 ANSWER 33 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 204975-30-4 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(aminomethyl)-2,3,5,6-tetramethylphenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C32 H40 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



Searched by M. Smith



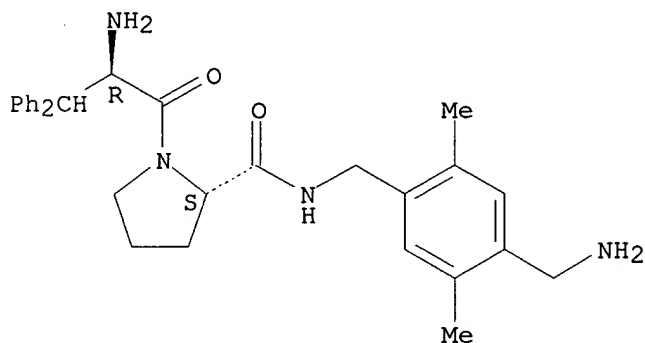
## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:238973

L5 ANSWER 34 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 204975-29-1 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(aminomethyl)-2,5-dimethylphenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C30 H36 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 128:238973

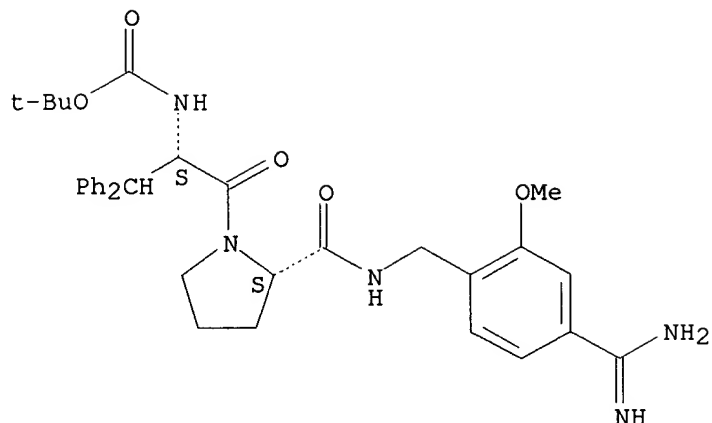
L5 ANSWER 35 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182292-32-6 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-L-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, diacetate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H41 N5 O5 . 2 C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 182292-31-5  
CMF C34 H41 N5 O5

Absolute stereochemistry.

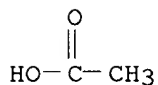
Searched by M. Smith



CM 2

CRN 64-19-7

CMF C2 H4 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 36 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 182292-31-5 REGISTRY

CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-L-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C34 H41 N5 O5

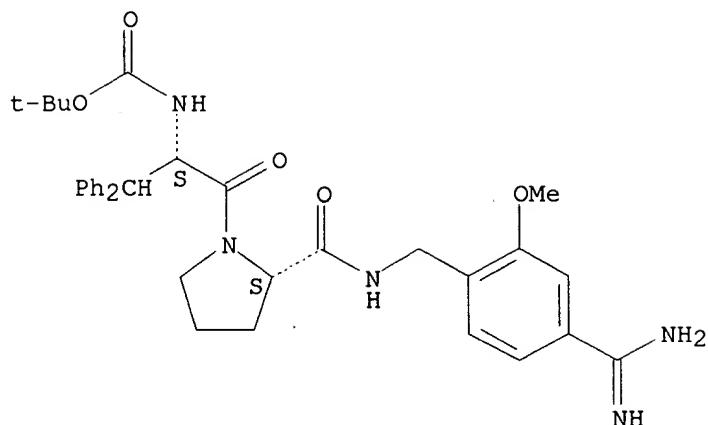
CI COM

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Searched by M. Smith



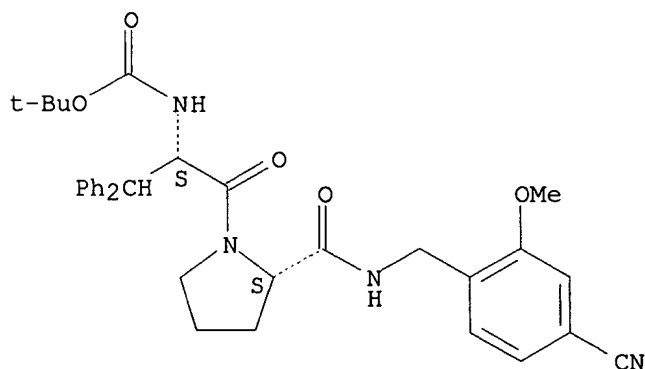
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 37 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182292-30-4 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-L-phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H38 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

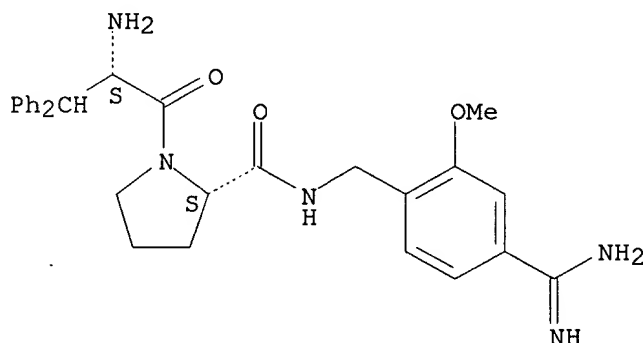
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

Searched by M. Smith

REFERENCE 1: 125:301605

L5 ANSWER 38 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182292-29-1 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-L-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H33 N5 O3 . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



● 2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

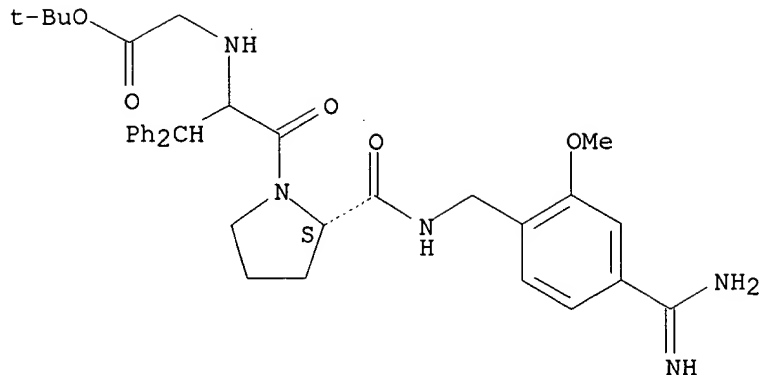
L5 ANSWER 39 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182290-33-1 REGISTRY  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monoacetate (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monoacetate  
FS STEREOSEARCH  
MF C35 H43 N5 O5 . C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 182290-32-0  
CMF C35 H43 N5 O5

Absolute stereochemistry.

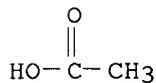
Searched by M. Smith



CM 2

CRN 64-19-7

CMF C2 H4 O2



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 40 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 182290-32-0 REGISTRY

CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-  
phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]- (9CI)  
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenyl-DL-  
phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-

FS STEREOSEARCH

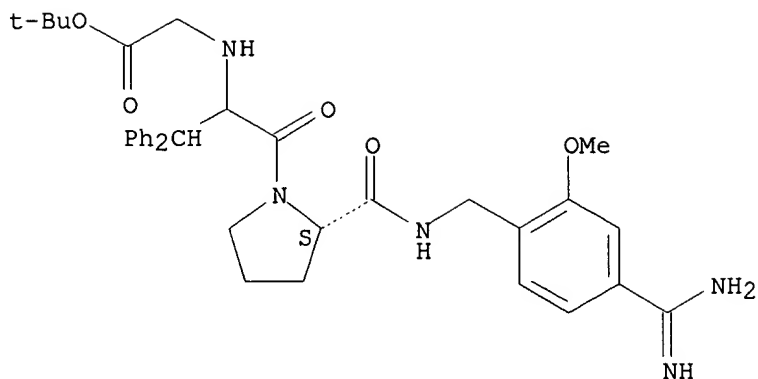
MF C35 H43 N5 O5

CI COM

SR CA

Absolute stereochemistry.

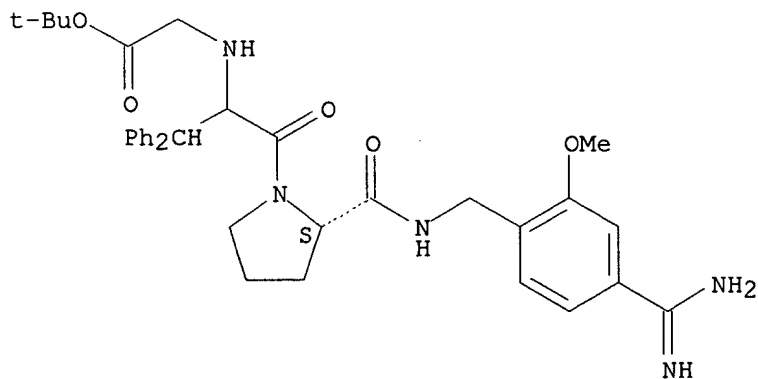
Searched by M. Smith



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 ANSWER 41 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182290-31-9 REGISTRY  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monohydriodide (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monohydriodide  
FS STEREOSEARCH  
MF C35 H43 N5 O5 . H I  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
CRN (182290-32-0)

Absolute stereochemistry.



HI

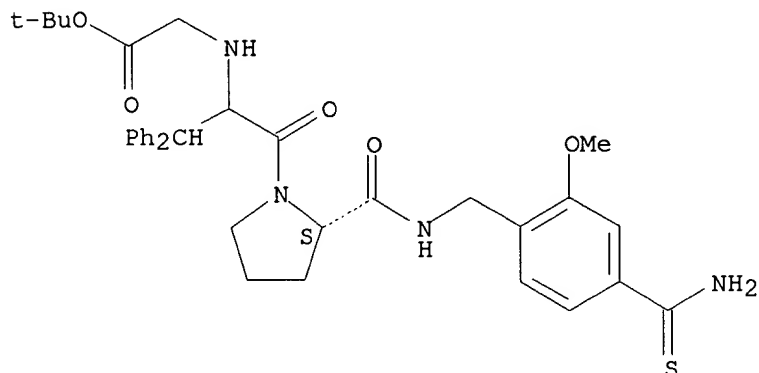
Searched by M. Smith

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 42 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182290-30-8 REGISTRY  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenylphenylalanyl-N-[[4-(aminothioxomethyl)-2-methoxyphenyl]methyl]-(9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminothioxomethyl)-2-methoxyphenyl]methyl]-  
FS STEREOSEARCH  
MF C35 H42 N4 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

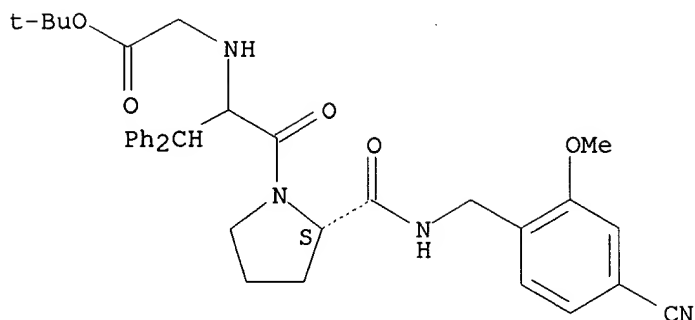
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 43 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182290-29-5 REGISTRY  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenylphenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-.beta.-phenyl-DL-phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-, monohydrochloride  
FS STEREOSEARCH  
MF C35 H40 N4 O5 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Searched by M. Smith



● HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

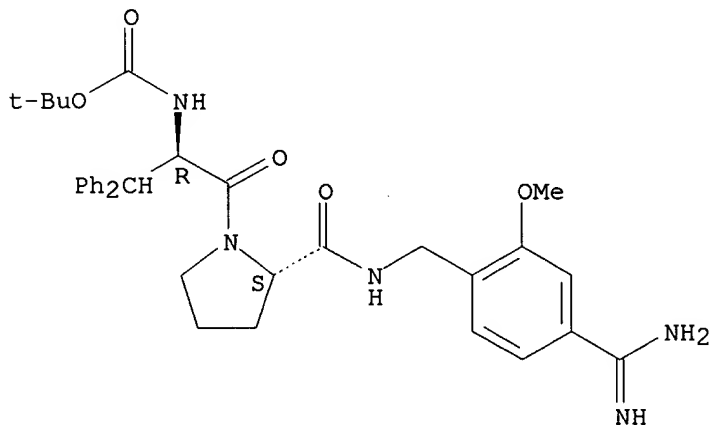
REFERENCE 1: 125:301605

L5 ANSWER 44 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182289-27-6 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, diacetate (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H41 N5 O5 . 2 C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 182289-25-4  
CMF C34 H41 N5 O5

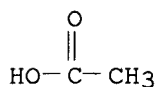
Absolute stereochemistry.



Searched by M. Smith



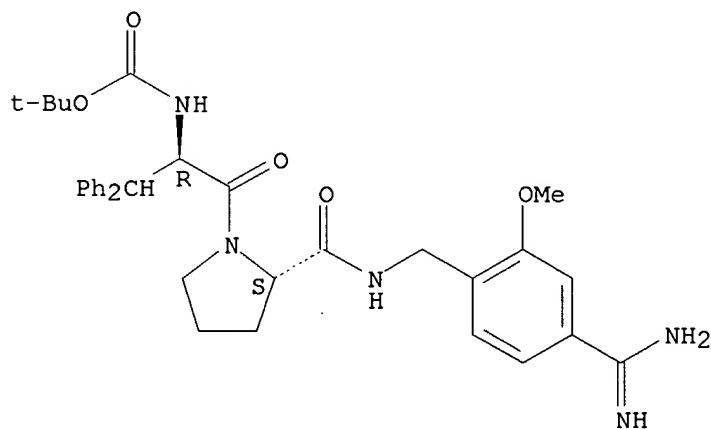
CM 2

CRN 64-19-7  
CMF C2 H4 O21 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 45 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182289-25-4 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H41 N5 O5  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

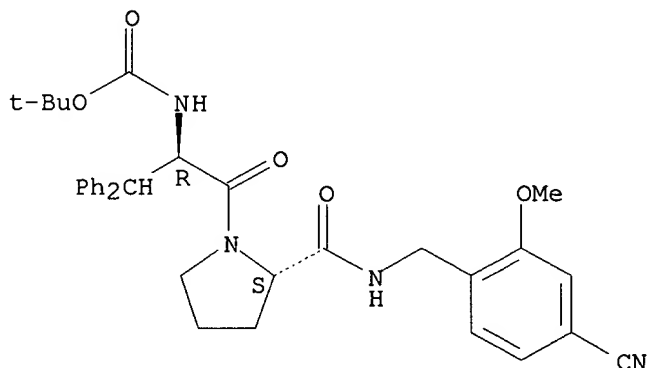
REFERENCE 1: 125:301605

L5 ANSWER 46 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182289-23-2 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-D-

Searched by M. Smith

phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H38 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

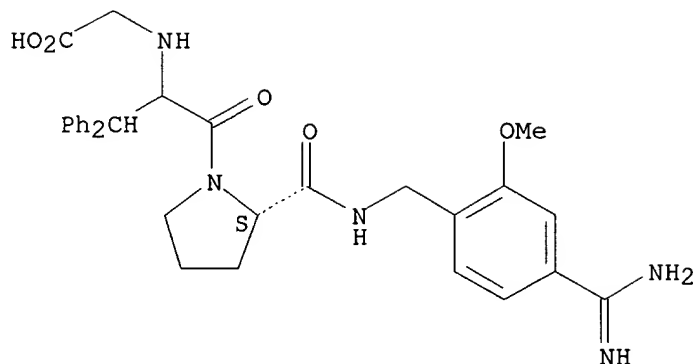
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 47 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182286-65-3 REGISTRY  
CN L-Prolinamide, N-(carboxymethyl)-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-(carboxymethyl)-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, dihydrochloride  
FS STEREOSEARCH  
MF C31 H35 N5 O5 . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

Searched by M. Smith



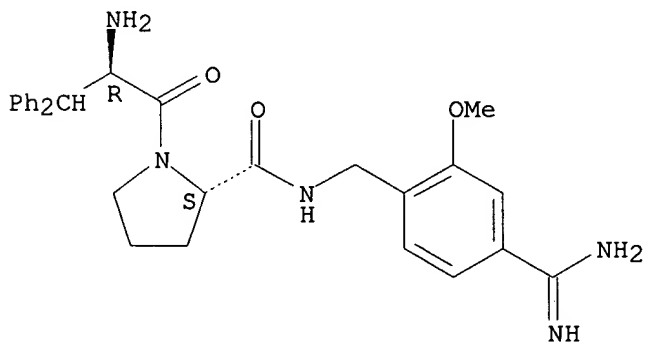
●2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

L5 ANSWER 48 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182286-35-7 REGISTRY  
CN L-Prolinamide, .beta.-phenyl-D-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H33 N5 O3 . 2 Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



●2 HCl

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:301605

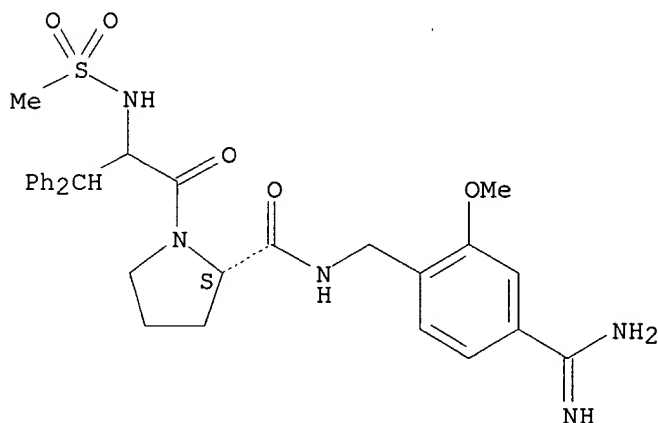
Searched by M. Smith

L5 ANSWER 49 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182159-36-0 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monohydriodide (9CI) (CA INDEX NAME)

## OTHER CA INDEX NAMES:

CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monohydriodide  
FS STEREOSEARCH  
MF C30 H35 N5 O5 S . H I  
SR CA  
LC STN Files: CA, CAPLUS  
CRN (182158-96-9)

Absolute stereochemistry.



● HI

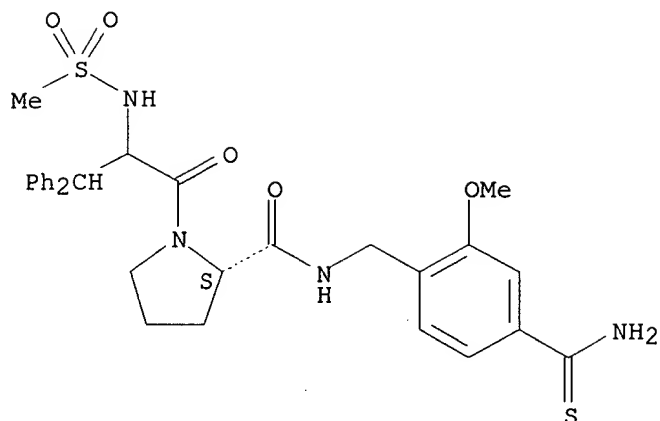
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585

L5 ANSWER 50 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182159-35-9 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenylphenylalanyl-N-[[4-(aminothioxomethyl)-2-methoxyphenyl]methyl]- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminothioxomethyl)-2-methoxyphenyl]methyl]-  
FS STEREOSEARCH  
MF C30 H34 N4 O5 S2  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by M. Smith



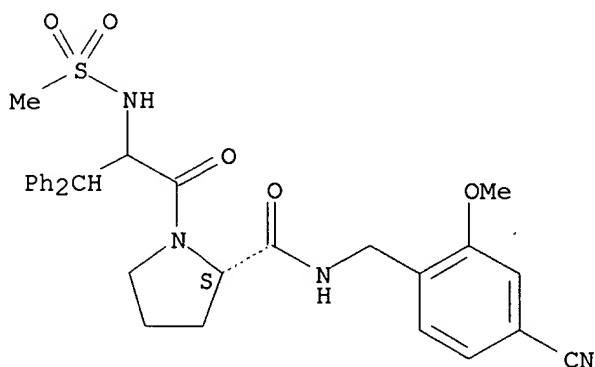
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585

L5 ANSWER 51 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182159-34-8 REGISTRY  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenylphenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-DL-phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-  
FS STEREOSEARCH  
MF C30 H32 N4 O5 S  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

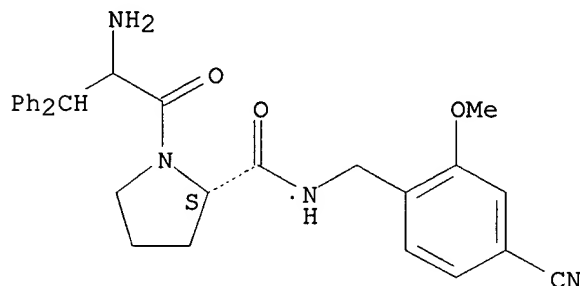
Searched by M. Smith

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585

L5 ANSWER 52 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182159-33-7 REGISTRY  
CN L-Prolinamide, .beta.-phenylphenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, .beta.-phenyl-DL-phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-, monohydrochloride  
FS STEREOSEARCH  
MF C29 H30 N4 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



● HCl

2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

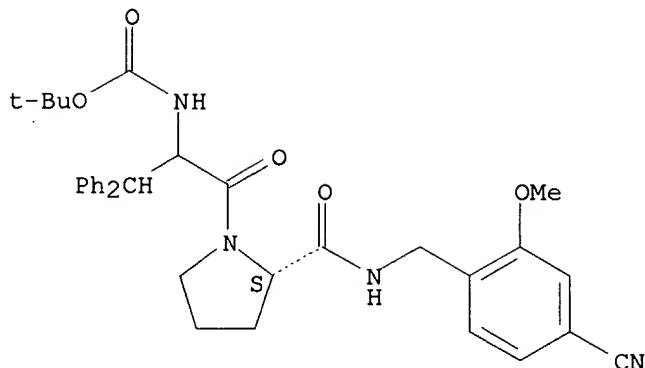
REFERENCE 1: 125:301605

REFERENCE 2: 125:276585

L5 ANSWER 53 OF 55 REGISTRY COPYRIGHT 2003 ACS  
RN 182159-32-6 REGISTRY  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenylphenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-.beta.-phenyl-DL-phenylalanyl-N-[(4-cyano-2-methoxyphenyl)methyl]-  
FS STEREOSEARCH  
MF C34 H38 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by M. Smith



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585

L5 ANSWER 54 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 182158-97-0 REGISTRY

CN L-Prolinamide, N-(methanesulfonyl)-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monoacetate (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN L-Prolinamide, N-(methanesulfonyl)-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-, monoacetate

FS STEREOSEARCH

MF C30 H35 N5 O5 S . C2 H4 O2

SR CA

LC STN Files: CA, CAPLUS

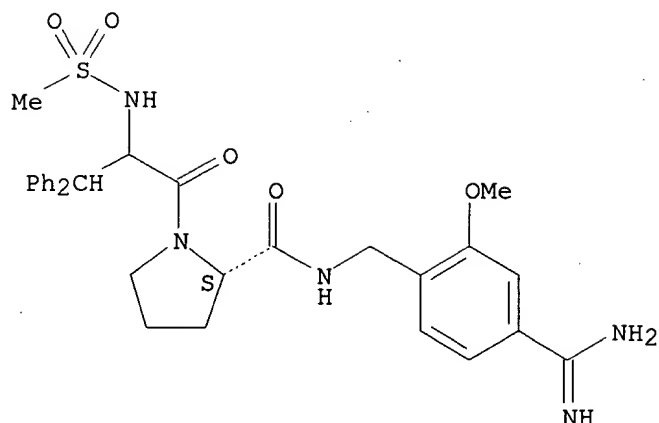
CM 1

CRN 182158-96-9

CMF C30 H35 N5 O5 S

Absolute stereochemistry.

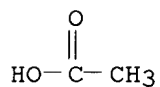
Searched by M. Smith



CM 2

CRN 64-19-7

CMF C2 H4 O2



1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585

L5 ANSWER 55 OF 55 REGISTRY COPYRIGHT 2003 ACS

RN 182158-96-9 REGISTRY

CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenylphenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN L-Prolinamide, N-(methylsulfonyl)-.beta.-phenyl-DL-phenylalanyl-N-[[4-(aminoiminomethyl)-2-methoxyphenyl]methyl]-

FS STEREOSEARCH

MF C30 H35 N5 O5 S

CI COM

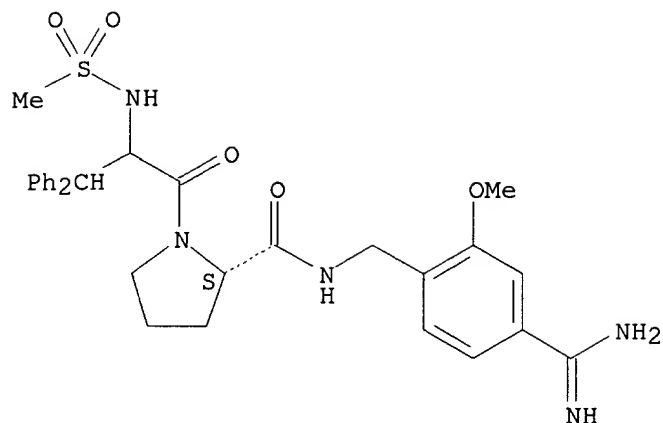
SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by M. Smith





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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:276585